# DIPPR Project 801 Evaluated Process Design Data

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### Introduction

DIPPR Project 801, Data Compilation, originated in the late 1970's as the flagship project of the Design Institute for Physical Property Data. Tom Daubert and Ron Danner of Penn State University were selected as the principal investigators of the project and the project has remained at Penn State since the project's inception. With Dr. Daubert's approaching retirement the steering committee of DIPPR 801 began a search in 1996 for a new contractor for the project and at the November 1996 AIChE meeting in Chicago awarded the contract to Brigham Young University with Richard Rowley, Vincent Wilding and John Oscarson as principal investigators. The project officially transfers January 1, 1998.

This paper reviews the history of Project 801 and looks to the future of the project.

# **History**

In the early to mid-1970's the need for accurate data for process design and simulation led to efforts to develop cooperative projects to develop thermophysical property databases. In other countries there were at the time government-sponsored database projects such as DECHEMA in Germany, but these projects did not satisfy the needs of industry in the U.S. due to difficulties of distance, lack of access to source data, and lack of industry involvement. Although some companies were pooling their efforts in small cooperative consortia, there was not an industry-wide, comprehensive undertaking in the United States [1, 2].

As part of his work in the mid 1970's to revise his book on physical property predictions, Professor Robert Reid invited a few companies to submit to him their physical property databases to potentially be combined into a single database in the book. Although there was reluctance on the part of these companies to share their databases, several agreed on conditions of confidentiality and anonymity. Professor Reid met with representatives of these companies at the November 1975 AIChE meeting and through the use of anonymous graphs of some of the data illustrated that, although they all had excellent databases, each database had major errors. Significantly, the errors differed from company to company [3].

In 1976 the National Bureau of Standards, with encouragement from Union Carbide, invited industry representatives to Gaithersburg where Project Evergreen, a data compilation project similar to that being worked on by Professor Reid, was proposed. There was lively discussion at this meeting about issues of funding, principal investigators and the need for experimental measurements to be included in the effort. Although there was no clear consensus reached on the project structure or operations, there was agreement that cooperative data compilation was a good idea and the sooner such an effort was begun the better.

In January of 1977, the first International Conference on Properties and Phase Equilibria for Product and Process Design was held at Asilomar, California. This meeting provided the opportunity for relaxed discussion of data compilation ideas between industry representatives and

a variety of university faculty. These discussions led to formalized meetings to develop a cooperative data compilation effort. The first of these meetings was hosted by Allied Chemical Research Company in Morristown, New Jersey with David Roth conducting. Allied suggested that one of the first items of business should be the selection of an appropriate umbrella organization within which to operate the project and proposed the Manufacturing Chemists Association (MCA), which is now the Chemical Manufacturers Association, (CMA).

During 1977 three meetings were held at MCA headquarters in Washington D. C. at which the participants debated the form and scope of the project. Some representatives desired the project to produce data books, similar to the API data book, while other representatives preferred computer products. There were also debates about the types of experimental measurements that should be undertaken and who should do them. Despite disagreements on these issues there was agreement on the balloting procedure for project sponsors and on weighting factors based on company size [3].

Unsurmountable difficulties surfaced at the second of the MCA meetings, where it became obvious that whenever two or more members of the organization talked about anything, there would have to be MCA lawyers present. Also, MCA was proposing an annual overhead budget of \$100,000, which was much more money than the participating companies could afford. A different umbrella organization was needed, and David Palmer of Amoco approached Dr. F. J. Van Antweren and Dr. J.C. Forman (outgoing and incoming Executive Secretaries of AIChE) about the possibility of AIChE assuming this role.

The response from AIChE was positive, and at the third of the meetings held at MCA a proposal to join with AIChE was accepted by the group. In 1978 David Roth made a formal presentation to the AIChE Council and Dr. Al Larsen of Monsanto prepared by-laws both of which were accepted by the council. John Prados was appointed as the Council liaison to help with the organization of what would be called the Design Institute for Physical Property Data. Prados had the requisite skills to bring the different factions with their different points of view together and at the November 1978 AIChE meeting DIPPR was launched. David Roth was elected Chairman of the Administrative Committee, John Prados was elected Chairman of the Technical Committee and David Palmer was elected Vice-Chairman. The steering committee for the Data Compilation Project and other project chairmen were also elected.

The Data Compilation Project was central to all of DIPPR's purposes and so a special meeting was held in September 1979 (at NBS in Gaithersburg) to select the contractor for this project. The contract was awarded to Professors Tom Daubert and Ron Danner of the Pennsylvania State University. Later that year, contractors for other projects were selected. Funded work began in 1980 on the Data Compilation project and three other DIPPR projects.

## **Project 801 Today**

DIPPR 801 has been the largest DIPPR project both in terms of financial support and number of sponsoring companies. The early years of the project focused on adding compounds to the database, but as the number of compounds included in the database has increased more emphasis has been placed on systematic review of the data in the database. Presently, there are over 1700 chemicals included in the sponsor version of the database with 29 property constants and 15 temperature-dependent property correlations. Figures 1 and 2 show a typical data sheet (for water) from the database.

The objective of the DIPPR Data Compilation Project is to develop, organize, and make available to the project sponsors a complete, critically-evaluated compilation of thermophysical and transport properties of industrial important chemicals. Four operational concepts have been critical to the success of Project 801 [4]:

1) Industrial Sponsor Control. The steering committee is made up of thermophysical property experts from the sponsoring companies who are very active in the operations of the project. These individuals understand best the data needs of their companies. All procedural matters, such as correlation forms, property units, or properties to be included are discussed and voted on by the steering committee before they are implemented. The committee also determines the annual project budget and the project contractor.

The committee is divided into review panels that evaluate proposed information (data, correlations, estimations) to be included in the database. Only after mutual agreement between the review panels and the project staff is the change incorporated into the database.

- 2) Critical evaluation. There are many compilations of property data, but the 801 database is unique in its emphasis on the "best value" available. The database gives single values for property constants and single correlations for temperature dependent properties. The original sources are available in the database, but the listed value is the single best value as determined by the project staff and steering committee. The listed value may be derived from many experimental determinations or, when no reliable experimental data are available, estimated from tested correlations and prediction methods. The evaluation procedure is at the heart of the project, and the procedures and practices are rigorous and thorough to ensure that the best value is indeed selected based on available information.
- 3) Consistency. Not all of the properties in the database are independent. For those that are interdependent, such as the properties associated with vaporization (heat of vaporization, vapor pressure, boiling point and acentric factor) it has been a deliberate objective of the project to ensure that the values for these properties are consistent.
- 4) Completeness. To satisfy the needs for property data in process design and development it is important to have complete sets of data. The project strives to provide values for all properties

for all chemicals included in the database. Critically evaluated estimation methods are relied upon when experimental data are lacking. The only gaps in the compilation are for compounds for which estimation methods are inconsistent or for inapplicable properties such as vapor properties for inorganic salts.

The efforts over the past seventeen years by the Penn State staff and the project steering committee to apply these four principles in accomplishing the objectives of Project has produced what is arguably the best process design database in the world.

# The Future

At the start of 1998 DIPPR 801 moves from the Pennsylvania State University to Brigham Young University. The goal of the new project staff is to continue to improve the database to meet the needs of its industrial sponsors. There are several key objectives to ensure the continued success of Project 801:

1. Efficient Database Transfer. The project staffs from BYU and PSU met in May (1997) to begin the transfer of the project to BYU. At that meeting the methods used by PSU to collect and evaluate data, to enter data into the database, and to disseminate the results to the sponsors and to the publishers of public versions of the database were discussed. The software that is used by PSU to accomplish the various tasks of the project was also examined. Toward the end of 1997 the hard files which contain all of the information on the compounds and the evaluations that have been accumulated over the past 17 years will be moved to BYU. An up-to-date electronic version of the database will also be sent as soon as Penn State finishes their revisions for 1997.

Space for the project, already committed by the university, will be available by September 1, 1997. Once this space is acquired, it will be prepared to accommodate the project operations. A file server for the database has already been acquired and a second has been ordered. Other computers will be obtained later in the year. Two graduate students are currently working on computer projects to enhance the database. The Project Coordinator, a key individual in the success of the project, has been hired. The goal of the BYU staff is that there will be no interruption in service to the project sponsors and the work of maintaining and improving the database will continue smoothly.

2. Improve Existing Database. Using Microsoft ACCESS® the database will be made fully relational. A relational database permits sophisticated user-defined searches on properties, conditions, compounds, etc. For example, a search for all compounds with boiling points within a certain range could easily be performed. This search could also include additional conditions such as the requirement of a certain functional group. One of the graduate students mentioned above is working on this aspect of the project and a prototype of the relational database is already functioning.

Many project sponsors will want to continue to receive the database in its current format since they have software set up to interface with this format. The relational database is able to output the database in its current format. The database will maintain this backwards compatibility as long as the project sponsors desire it. It is expected, however, that as new capabilities are added to the database which can not be accommodated in its current, restricted format that format changes will be more desirable to the sponsors.

3. Extend Accessibility and Flexibility. A website will be established for access to the database by project sponsors. This will facilitate quick, flexible, and complete access to the database, raw data, staff evaluations of data, and recommendations. There will be immediate access to modifications and additions to the database. The flexibility of database access will be enhanced through the use of the website which will include graphical and computational capabilities. The combination of the website with the relational database will permit on-line searches of the database. Communications between the project staff and the steering committee will also be facilitated through the use of the Internet. There are also possibilities of individual sponsors establishing intranet access to the database for all users in their company.

The BYU staff developed a prototype website as part of the proposal process for Project 801. Although rudimentary in its capabilities, this website demonstrated some of the exciting possibilities of Internet access to the database. The second graduate student mentioned above is currently working on the design of the website. At this point communication between the website and the relational database has been established. The development of the website will continue for the next several months.

- 4. Augment the database. One of the main objectives of Project 801 has always been the addition of new compounds to the database. This work will continue with new compounds being added to the database at a rate of about 50 chemicals per year. The project sponsors develop the priority list of chemicals to be added each year. New properties will be added from time to time as approved by the steering committee. Some possibilities include molecular structure, safety, or environmental properties.
- 5. Maintain the database. Procedures for the efficient, accurate maintenance of the database will be implemented. Statistical process control concepts will be used to systematically eliminate errors in the database. Systematic reviews of the database will be performed in which the quality of the data will be evaluated, consistency tests will be performed, and new data will be incorporated into the database.

The correlations used to represent temperature dependent properties and the estimation methods used in the absence of reliable data will also be updated as better methods are developed. The project staff will be actively involved in development and evaluation of these methods.

#### Conclusion

The DIPPR 801 Project has been an extremely valuable undertaking for the industrial sponsors of the project and for all engineers and scientists who rely on the database. The operational philosophies that have made the project successful will continue to guide the project, and new capabilities and technologies will be added to ensure that the DIPPR 801 Evaluated Process Design Database continues to meet the needs of industry.

#### References

- 1. Thomson, G. H., A. H. Larsen, *DIPPR: Satisfying Industry Data Needs. J. Chem. Eng. Data* **1996**, *Vol. 41*, *No. 5*, 930-934.
- 2. Larsen, A. H., *Significance of the DIPPR Data Compilation.*, presented at the November 1982 AIChE National Meeting in St. Louis, Mo.
- 3. Palmer, D. A., DIPPR An Improbable Success. AIChE Symp. Ser. 1990, 86, No. 275, 1-4.
- 4. Buck, E., *Project 801: The DIPPR Data Compilation Project. AIChE Symp. Ser.* **1990**, 86, No. 275, 5-14.

#### PROPERTY CONSTANTS

Chemical Abstracts Name: WATER H20 IUPAC Name: WATER WATER Synonyms: DIHYDROGEN OXIDE ICE STEAM REFRIGERANT 718

Chemical Abstracts Number: 7732-18-5 Structural Formula: HOH

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PROPERTY	UNITS	VALUE	NOTE	QUAL CODE	ACCEPTED REFERENCE(S)	REJECTED REFERENCE(S)		
Molecular Weight Critical Temperature Critical Pressure Critical Volume Crit Compress Factor	kg/kmol K Pa m**3/kmol	18.015 647.13 2.2055E+07 .05595 .229		XE1 XE1 XE1 D	1 2909 2729 1886 2909 2984 2729 2909 1886 2984 PS	424 5 3	Ī	
Melting Point Triple Pt Temperature Triple Pt Pressure Normal Boiling Point Liq Molar Volume	K K Pa K m**3/kmol	273.15 273.16 6.1173E+02 373.15 .018069		XE1 XE1 XE1 XE1 XE1	424 2729 3 424 48 2909 2909 424 1319 2909 424 2729 2909 424 3			
IG Heat of Formation IG Gibbs of Formation IG Absolute Entropy Std Heat of Formation *Std Gibbs of Formation	J/kmol J/kmol J/kmol*K J/kmol J/kmol	-2.4181E+08 -2.2859E+08 1.8872E+05 -2.8583E+08 -2.3717E+08	1 2	XE1Z D 1 XE1Z XE1 D 2	1314 1124 47 PS 1124 48 1314 1124 3658 PS PS			
*Std Absolute Entropy Heat Fusion at Melt Pt Std Net Heat of Comb Acentric Factor Radius of Gyration	J/kmol*K J/kmol J/kmol m	7.0390E+04 6.0017E+06 0.0 .3449 6.1500E-11	3 4	P 2 XE1Z D D 3	PS 424 48 PS PS 43 11 11 12	22		
Solubility Parameter Dipole Moment van der Waals Volume van der Waals Area Refractive Index	(J/m**3)**.5 C*m m**3/kmo1 m**2/kmo1	4.7810E+04 6.1700E-30 .01237 2.2600E+08 1.3325	5 6	D 3 XE2Z D 3 D 4 XE1	PS 25 1518 72 389 1092 43 8			
Flash Point Flammability Limits Flamm Limit Temps Autoignition Temp	K vol % K K		7 7 7				Ī	

Issue Date: JULY 1981 Revision Date: AUG. 1996

- NOTES: 1. Calculated from the enthalpy of formation and the absolute entropy. 2. Calculated from the standard state enthalpy of formation and the standard state absolute entropy.
  - 3. Calculated from ideal gas absolute entropy.
  - 4. Product of combustion.

  - 5. Do not use this value to calculate r for the UNIQUAC equation.
    6. Estimated by method of Vera, et al. Do not use to calculate
  - q for the UNIQUAC equation.
  - 7. Property inappropriate for this substance.

CONST.

H20

Figure 1. Property Constants for Water.

Chemical Abstracts Name: W	ATER							H2O WATER
Property   NTE   EQN   Q   COEFFICIENTS								
1				A	В	C	D	E
Solid Density   Min( 233.15, 5.1202E+01)   Max( 273.15, 5.0888E+01)		100	2	5.3030E+01	-7.8409E-03			
Liquid Density Min( 273.16, 5.5846E+01) Max( 647.13, 1.8060E+01)		116	3	1.8060E+01	2.5309E+01	6.6173E+01	-5.0206E+01	
*Solid Vapor Pressure Min( 149.30, 5.5487E-06) Max( 273.16, 6.1403E+02)		101	1	3.5169E+01	-6.1494E+03	-1.3785E+00	5.4788E-03	1.0000E+00
Vapor Pressure Min( 273.16, 6.1056E+02) Max( 647.13, 2.1940E+07)		101	1	7.3649E+01	-7.2582E+03	-7.3037E+00	4.1653E-06	2.0000E+00
Heat of Vaporization Min( 273.16, 4.4733E+07) Max( 647.13, 0.0000E+00)		106	2	5.2053E+07	3.1990E-01	-2.1200E-01	2.5795E-01	
Solid Heat Capacity Min( 3.15, 1.8015E+02) Max( 273.15, 3.8121E+04)		100	3	-2.6249E+02	1.4052E+02			
Liquid Heat Capacity Min( 273.16, 7.6150E+04) Max( 533.15, 8.9394E+04)		100	2	2.7637E+05	-2.0901E+03	8.1250E+00	-1.4116E-02	9.3701E-06
Ideal Gas Heat Capacity Min( 100.00, 3.3363E+04) Max(2273.15, 5.2760E+04)		107	2	3.3363E+04	2.6790E+04	2.6105E+03	8.8960E+03	1.1690E+03
Second Virial Coefficient Min( 273.15,-1.7827E+00) Max(2273.10, 9.1885E-03)		104	4	2.2220E-02	-2.6380E+01	-1.6750E+07	-3.8940E+19	3.1330E+21
Liquid Viscosity Min( 273.16, 1.7016E-03) Max( 646.15, 5.0277E-05)		101	3	-5.2843E+01	3.7036E+03	5.8660E+00	-5.8790E-29	1.0000E+01
Vapor Viscosity Min( 273.16, 8.9078E-06) Max(1073.15, 4.0603E-05)		102	2	6.1839E-07	6.7779E-01	8.4723E+02	-7.3930E+04	
*Solid Thermal Conductivity Min Max	2							
Liq Thermal Conductivity Min( 273.16, 5.6716E-01) Max( 633.15, 4.2715E-01)		100	2	-4.3200E-01	5.7255E-03	-8.0780E-06	1.8610E-09	
Vap Thermal Conductivity Min( 273.16, 1.7019E-02) Max(1073.15, 1.0748E-01)		102	2	2.1606E-03	7.6839E-01	3.9405E+03	-4.4534E+05	
Surface Tension Min( 273.16, 7.7919E-02) Max( 647.13, 0.0000E+00)		106	2	1.8548E-01	2.7170E+00	-3.5540E+00	2.0470E+00	

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1. For the short temperature range 273.16 to 333.15 K using equation 100, use the following coefficients: A - 1.3851E+01, B = 6.4038E-01, C = -1.9124E-03, and D = 1.8211E-06.

2. No experimental values or satisfactory prediction method available. NOTES: 1.

PROPERTY	ACCEPTED REFERENCES     USED IN REGRESSION   NOT USED IN REGRESSION							 <u> </u> 	REJECTED REFERENCES
Solid Density   Liquid Density   Solid Vapor Pressure	424 2909 509	424	48 47	174	424				
Vapor Pressure   Heat of Vaporization   Solid Heat Capacity	2909 2909 174		47 175	175 1348				1932	
Liquid Heat Capacity Ideal Gas Heat Capacity Second Virial Coefficient	2909 2909 2909		174 424 3	47 890		1611 4143		3	
Liquid Viscosity  Vapor Viscosity  Solid Thermal Conductivity	3830 2909 3	8830	175 174	47 2416		2416	2909		
Liq Thermal Conductivity  Vap Thermal Conductivity	3830 2909 3	8830	!	2659		1976	2659		
Surface Tension	2909		6	1961				33	

Figure 2. Temperature-Dependent Correlation Coefficients for Water.